



- Gregory Stella, U.S. EPA
 - Environmental Engineer
 - Emission Factor and Inventory Group
 - Primary Roles
 - Preparation of Inventories for Emissions Modeling
 - Emissions Modeling Support for Regulatory Actions
 - International Emissions Inventory Coordination
 - Emission Projection and Projection Tools



- Marty Wolf & Paula Fields
 - Eastern Research Group (ERG)
- Graphics Provided From
 - "Mexico Emissions Inventory Program
 Manuals; Volume VIII Modeling Inventory
 Development"
 - http://www.epa.gov/ttn/catc/dir1/modeldev.pdf

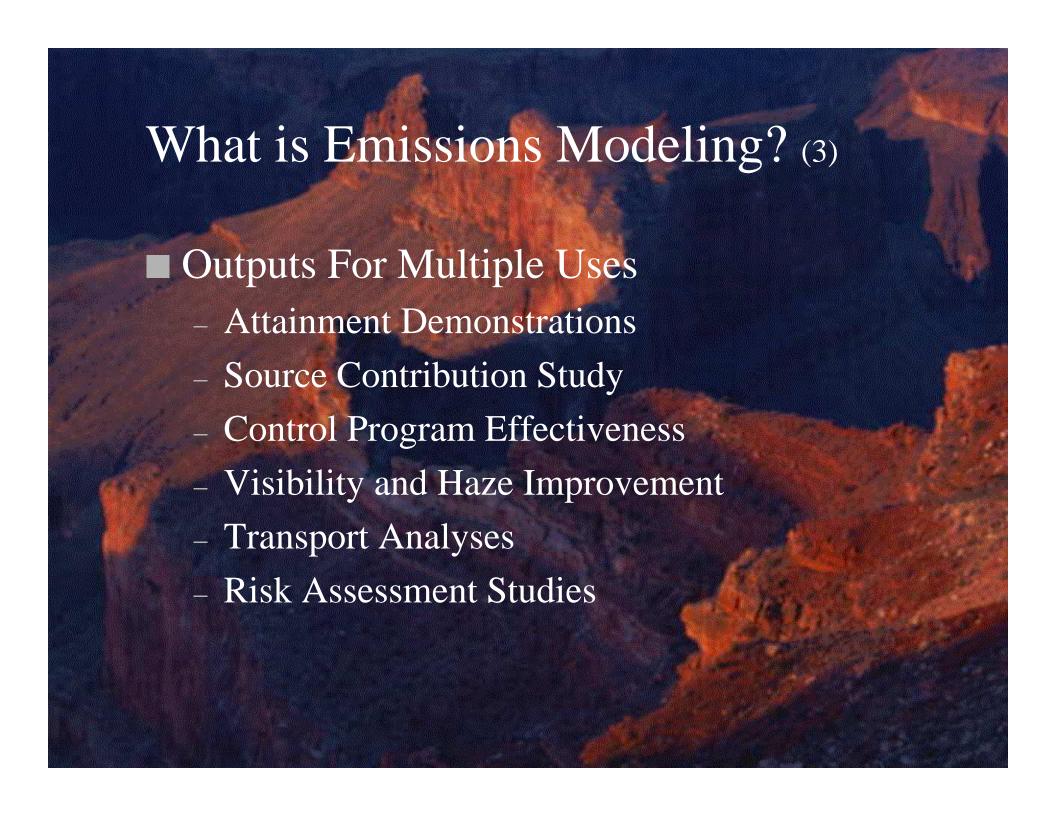


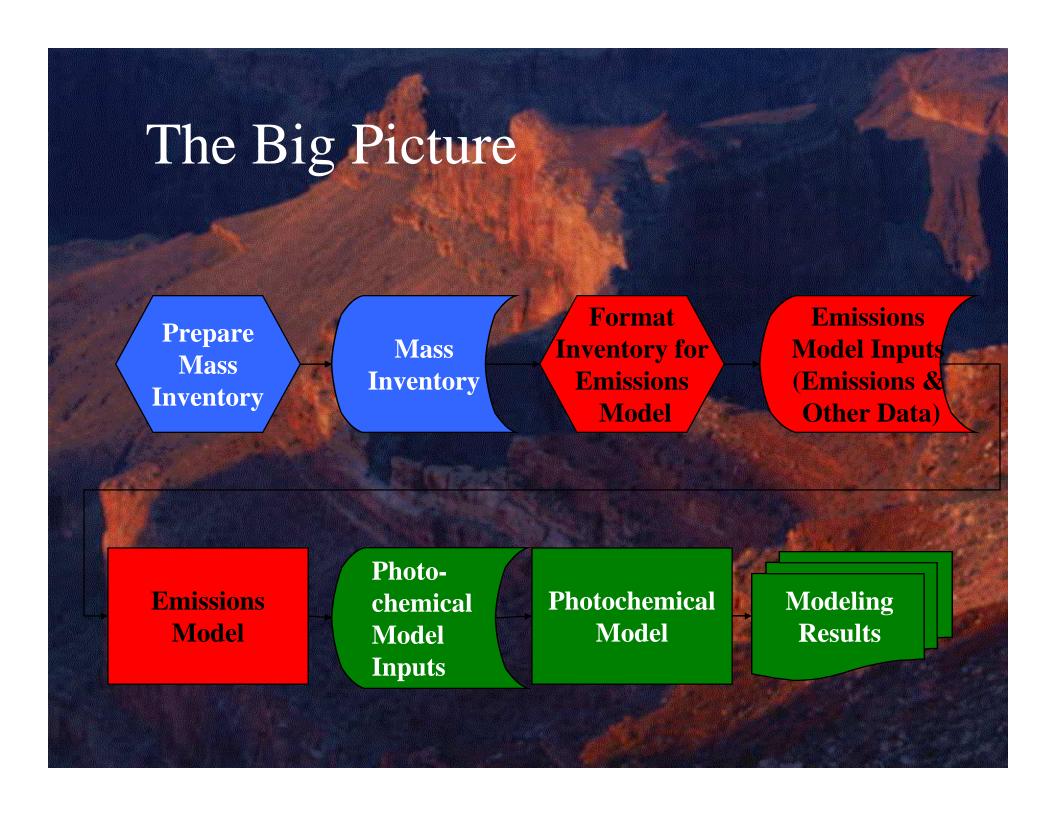
 The Translation of a Mass Inventory Into an Inventory Ready for Input Into an Air Quality Model

Mass Inventory Which Can Support Temporal, Spatial, Speciation, and Projection Needs



- Providing Detailed Emission Inventory Plan
 - Location
 - Release Times / Frequency
 - Process Types
- Combining with Meteorological Data
- Modeling Complex Chemical Interactions and Transport Activity

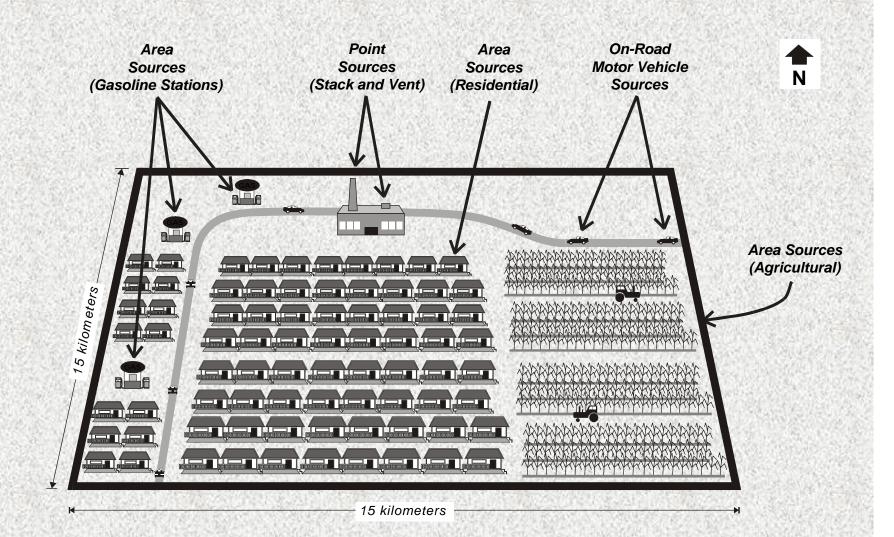






- Gridded Emissions
 - Surface Layer/Elevated
- Speciated Emissions
- Temporally Allocated Emissions
- Projected and Controlled Emissions
- Generally Contains No Specific Information
 - Plant IDs, SCC, Etc.

Example Modeling Domain

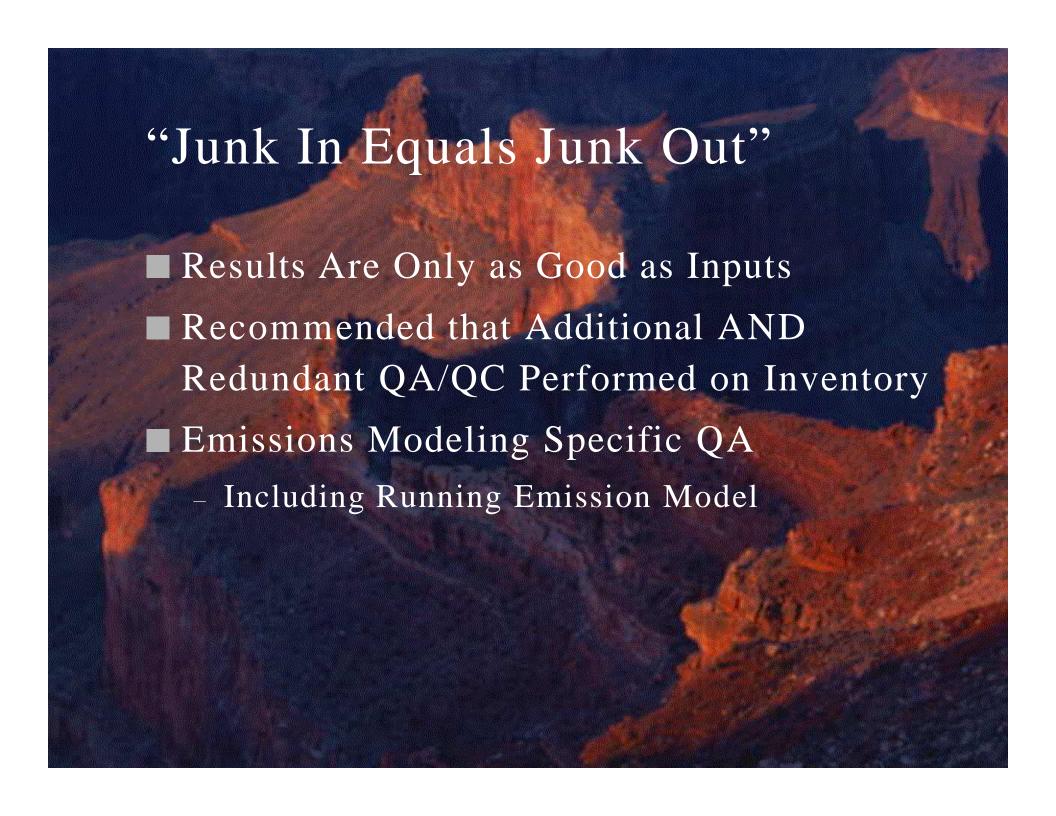


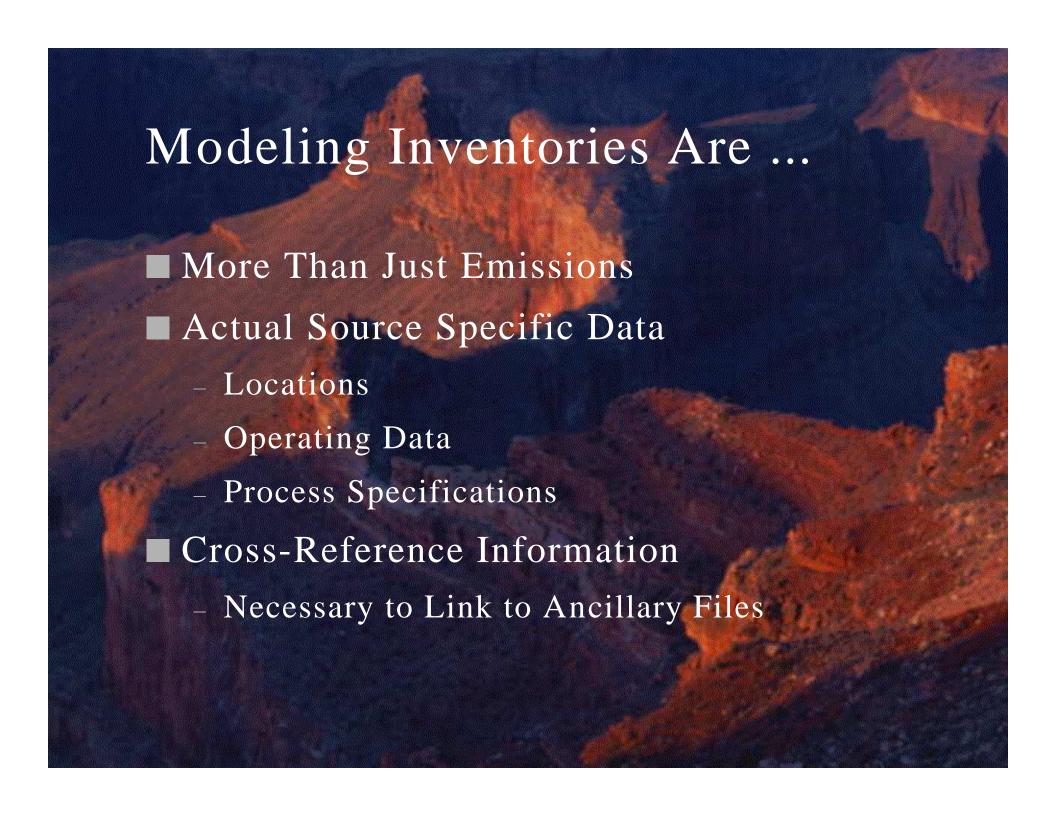
Example Domain Emissions

Emission Source	Annual Emissions (Tons/yr)		
	VOC	NOx	CO
Point Sources			
Factory (Boiler)	200	400	600
Factory (Surface Coating)	300	0	0
Mobile Sources			
Automobiles	400	800	600
Area Sources			
Gasoline Stations	150	0	0
Residential Commercial Solvent Use	200	0	0
Agricultural Pesticide Application	100	0	0











- Hourly Time Resolution
- Gridded Emissions (Vertical & Horizontal)
- Chemical Species To Match AQ Chemistry
- All Source Type Emissions
 - Anthropogenic, Biogenic, Geogenic
- Domain Wide Coverage
- Process & Control Information

Why Such Detail?

- Source Distance Relative to Receptors
- Many Sources Have Significant Temporal Variation in Emission Rates
- Different Processes Have Varying Reactivities and Volatilities
- Release Heights Have Transport and Diffusion Characteristics
- Data Used as Surrogates or Cross-Reference



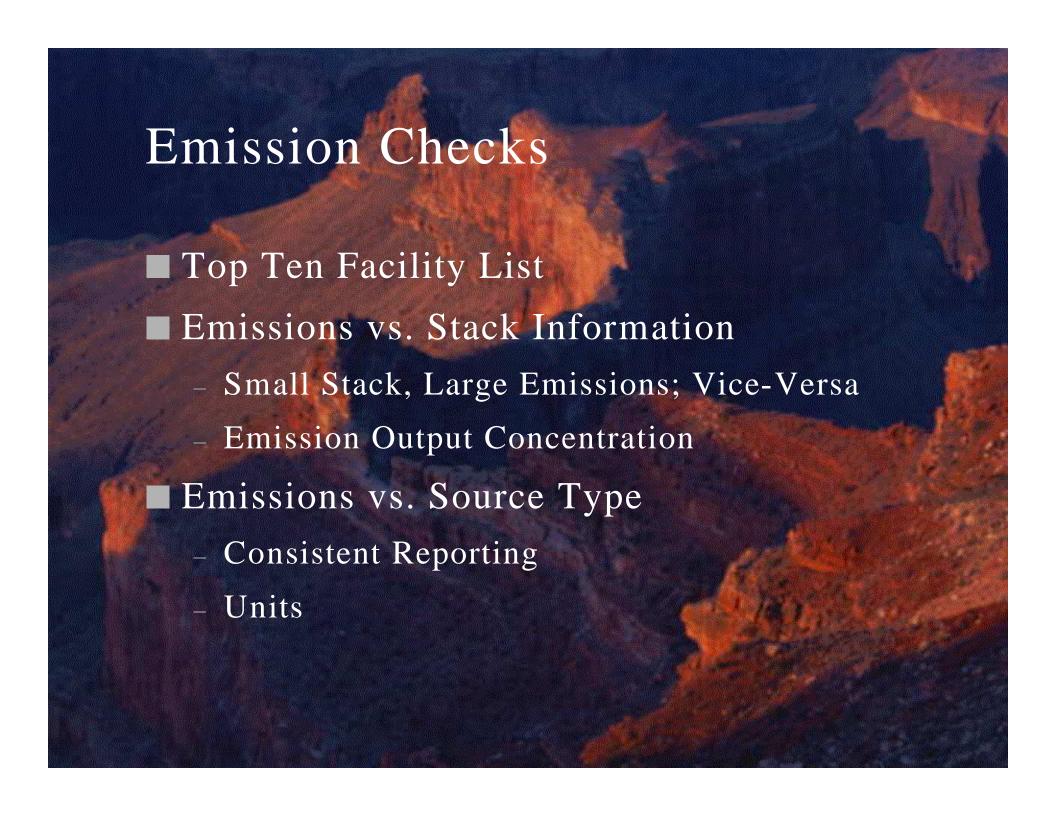
- Required for Modeling
 - Process Level Emissions
 - Geographic Coordinates
 - Stack Parameters
 - Operating Schedule
- Additional Projection Needs
 - SIC
 - Activity
 - Emission Factors (Control Efficiency)



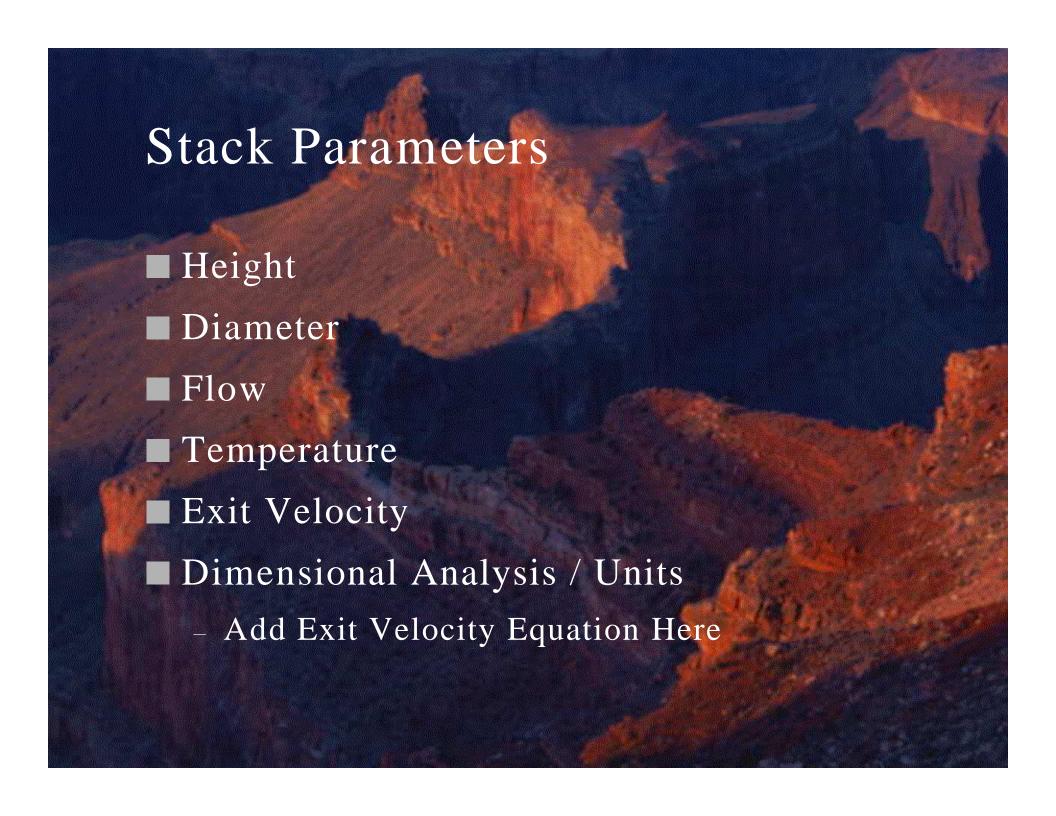


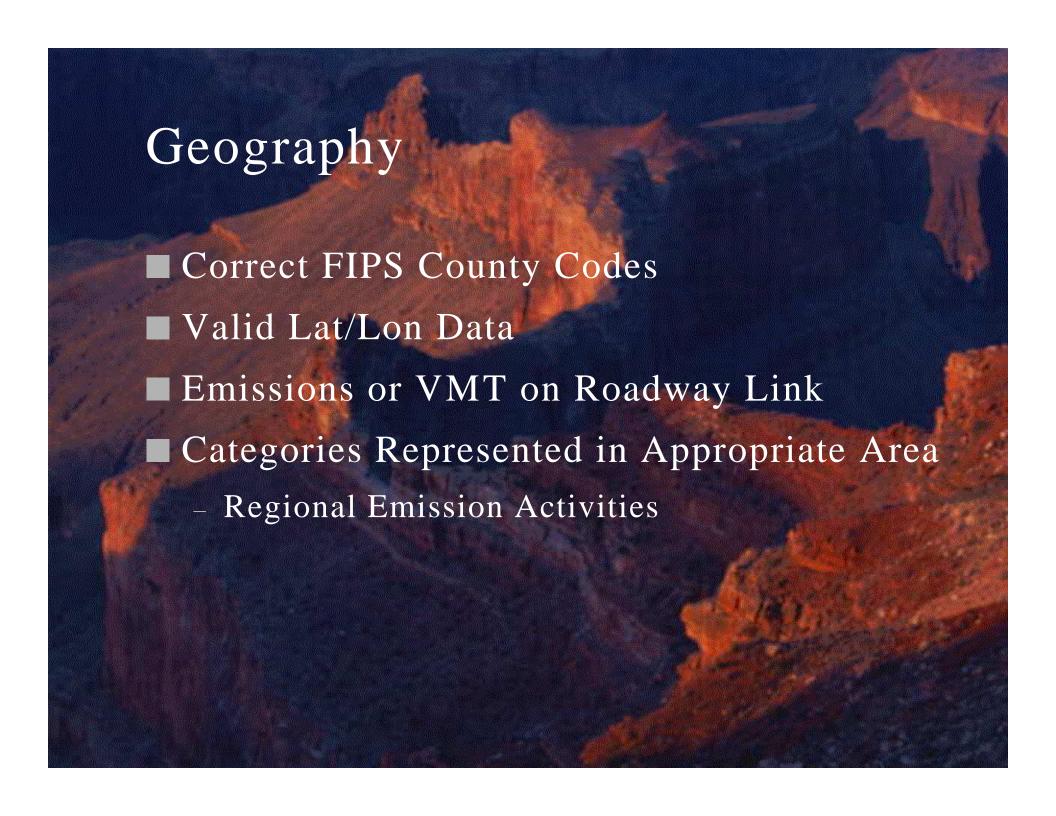


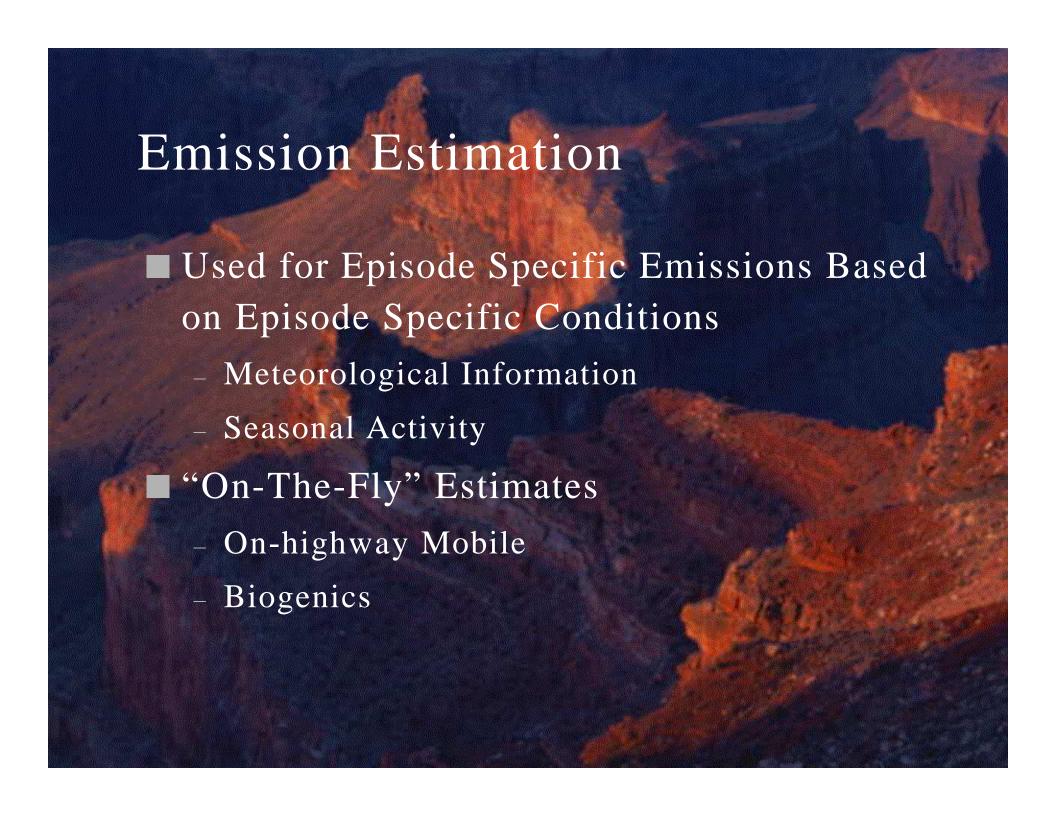
- Compare Sources and Source Types to Previous Years
 - Are Same Facilities in Operation?
 - Are Same Source Types Represented?
- Compare Emissions to Sources of Same Type
 - Are Emissions Comparable?
 - Are All Source Types Represented?

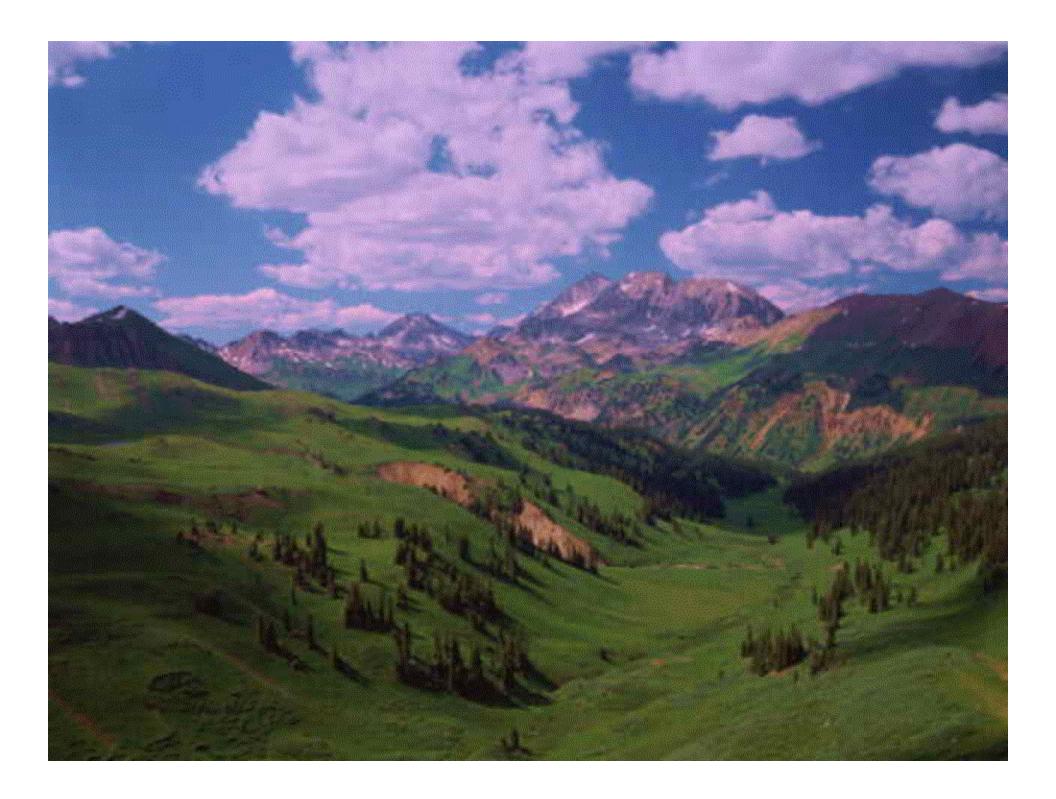














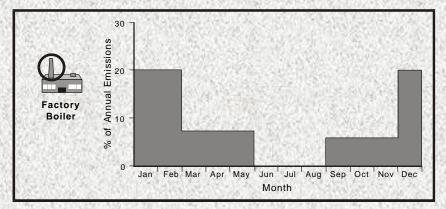
- Allocation of Emissions to Time-Period Required by Model
 - Annual or Daily Emissions to Hourly Emissions
- Use Operating Schedule Data and Default Temporal Profiles
 - Actual Hours, Days, Weeks, Seasonal Data

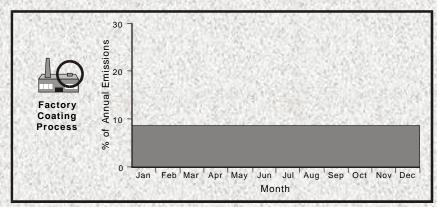


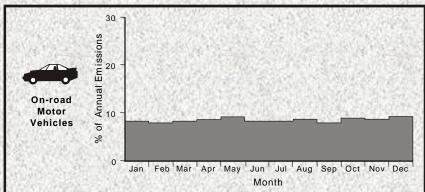
- Monthly or Seasonal Allocation
 - April, Summer, Ozone Season, etc.
- Weekly Allocation
 - Average Day, Wednesday, Sunday, etc.
- Hourly Allocation
 - 8 AM, Noon, 6 PM, etc.
- Holiday Allocation
 - 4th of July, Labor Day, Christmas, etc.

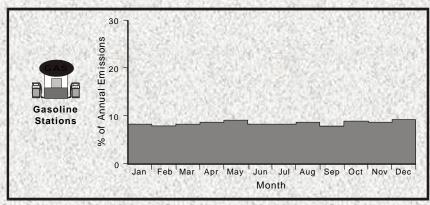


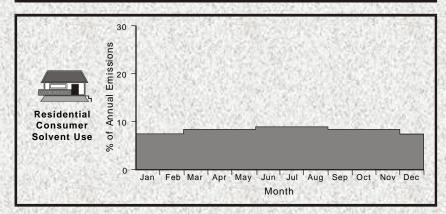
- Used to Generate Seasonal or Monthly Emission and Activity Estimates
- Combinations of Months Used for Seasons
 - Spring (Mar, Apr, May)
 - Summer (Jun, Jul, Aug)
 - Fall (Sep, Oct, Nov)
 - Winter (Dec, Jan, Feb)

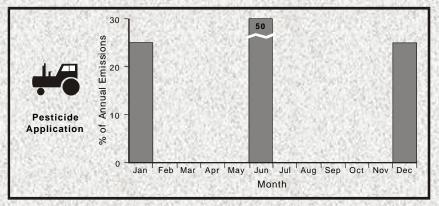












Seasonal Temporal Allocation

■ Example:

Calculate Spring NOx Emissions from Factory
 Boiler in Example Domain

■ Steps:

- Estimate Seasonal Allocation Factor from Monthly Profiles
- Apply Seasonal Allocation Factor to Annual Emissions

Seasonal Temporal Allocation

Calculate Spring Allocation Factor

$$AF_{Spr} = AF_{Mar} + AF_{Apr} + AF_{may}$$

AF_{Spr} = Spring Temporal Allocation Factor

AF_{Mar} = March Temporal Allocation Factor

AF_{Apr} = April Temporal Allocation Factor

AF_{Mav} = May Temporal Allocation Factor

Seasonal Temporal Allocation (2)

■ From Seasonal Allocation Profiles

$$AF_{Spr} = 0.073 + 0.073 + 0.073$$

 $AF_{Spr} = 0.219$

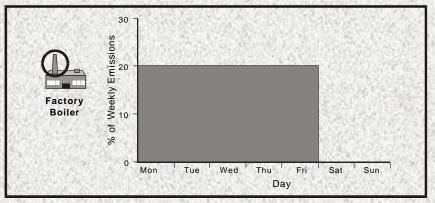
Apply Spring Factor to Annual Emissions

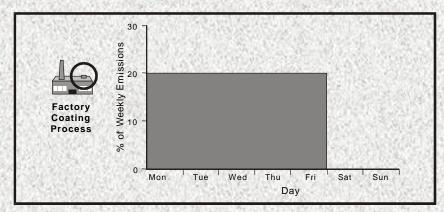
$$E_{Spr} = E_{Ann} * AF_{Spr}$$

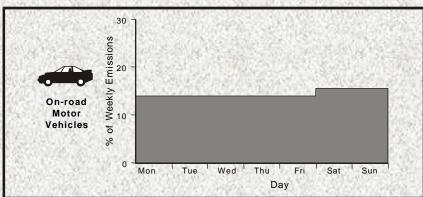
 $E_{Spr} = 400 \text{ Tons NOx/yr * 0.219}$
 $E_{Spr} = 87.6 \text{ Tons NOx}$

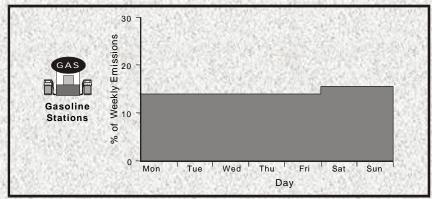


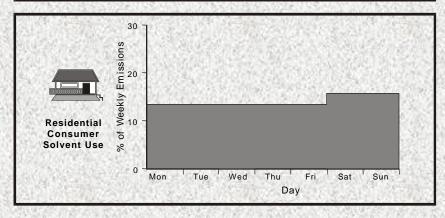
- Used to Generate Specific Day or Day Type
 Emission and Activity Estimates
- Most Sources Are Not Constant Emitters
 - Weekday vs. Weekend Differences
 - Specific Day of Week
 - Mon, Tues, Wed, etc.
 - Recreational Activities
 - More on Weekends

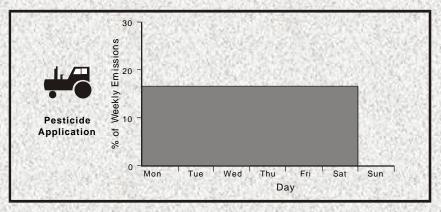












Weekly Temporal Allocation

■ Example:

 Calculate Average Thursday NOx Emissions from Factory Boiler in Example Domain

■ Steps:

- Estimate Average Thursday Allocation Factor from Weekly Profiles
- Apply Average Thursday Allocation Factor to Seasonal Emissions

Weekly Temporal Definitions

- Average Daily Factor (AF_{ADay})
 - Contribution of Any One Day to Season
 - 1.00 / 91 days per season
- Average Daily Activity (AC_{Day})
 - Percentage of Ave Day Activity for Week
 - 1.00 / 7 days per week
- Specific Day Activity (AC_{SpecDay})
 - Percentage of Specific Day Activity for Week

Weekly Temporal Allocation

■ Calculate Average Thursday Allocation Factor

$$AF_{Thur} = AF_{ADay} * (AC_{Thur} / AC_{Day})$$

AF_{Thur} = Thursday Allocation Factor

AF_{ADay} = Average Daily Factor

AC_{Thur} = Thursday Activity Factor

AC_{Day} = Average Daily Activity Factor

Weekly Temporal Allocation (2)

■ From Weekly Allocation Profiles

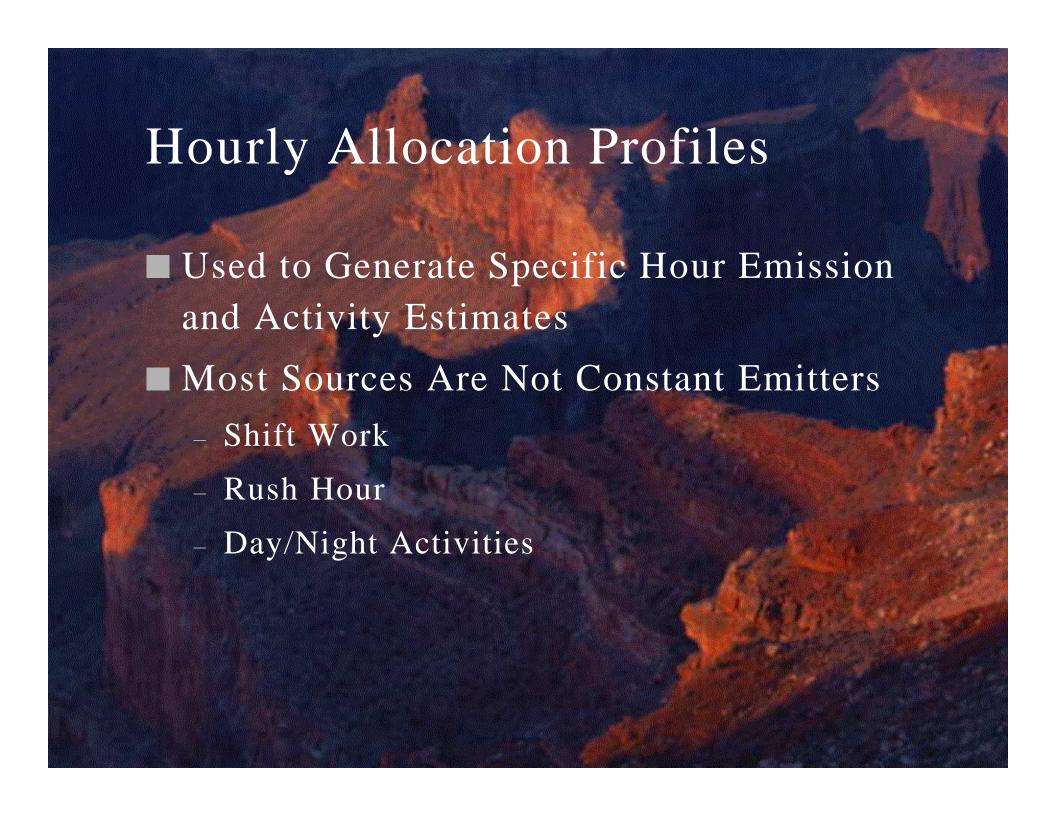
$$AF_{Thur} = (1/91) * (0.200/0.1429)$$

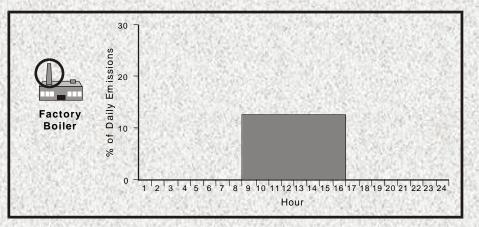
= 0.0154

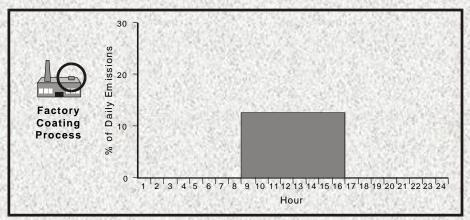
Apply Thursday Factor to Season Emissions

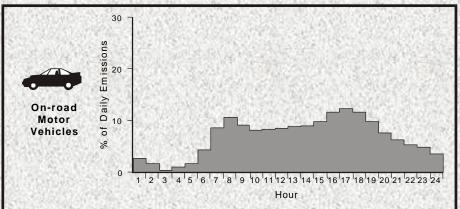
 $E_{Thur} = E_{Spr} * AF_{Thur}$ $E_{Thur} = 87.6 \text{ Tons NOx/Spring * 0.0154}$

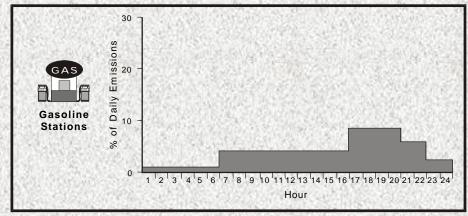
 $E_{Thur} = 1.35$ Tons NOx/ Spring Thursday

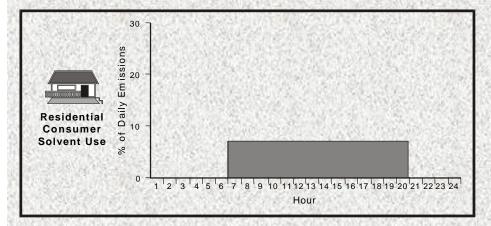


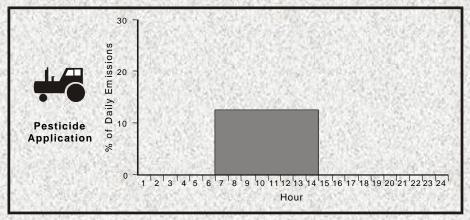












Hourly Temporal Allocation

■ Example:

 Calculate 2:00 P.M. NOx Emissions from Factory Boiler in Example Domain

■ Steps:

- Estimate 2:00 P.M. Allocation Factor from Hourly Profiles
- Apply Hourly Allocation Factor to Daily Emissions



■ Calculate Hourly Allocation Factor

 $AF_{Hour} = AC_{Hour} / AC_{Day}$

AF_{Hour} = Hourly Allocation Factor

AC_{Hour} = Hour Specific Activity

 $AC_{Day} = Daily Activity$

Hourly Temporal Allocation (2)

■ From Hourly Allocation Profiles

$$AF_{2PM} = 0.125/1.00$$

= 0.125

Apply Hourly Factor to Daily Emissions

 $E_{2PM} = E_{Thur} * AF_{2PM}$

 $E_{2PM} = 1.35$ Tons NOx/Thursday * 0.125

 $E_{2PM} = 0.1688$ Tons NOx/ 2PM Spring Thursday

Temporal Allocation Issues

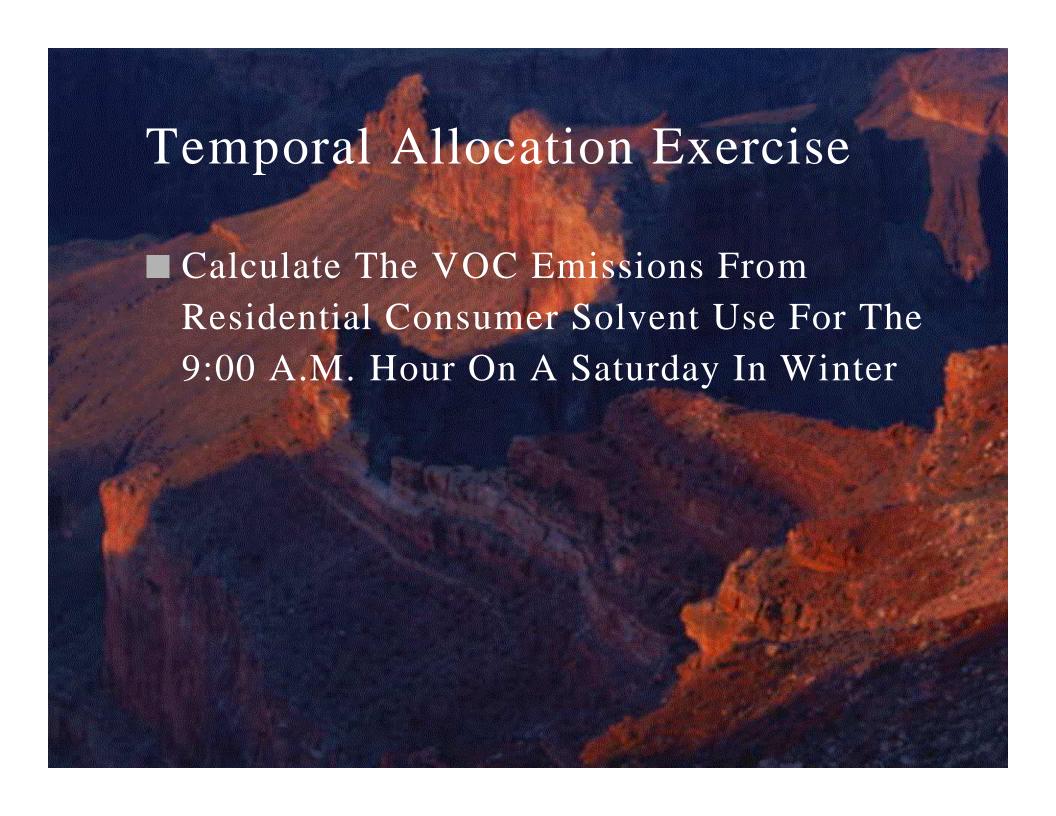
- Majority of Submitted Data Fall into Uniform Daily and Hourly Profiles
 - 24 hours/day, 7 days/week
- Can Use Hourly Emissions If Available
 - CEM, Other Monitored Sources
- PM/Visibility Modeling Will Require Emissions for Winter, Spring, Summer, and Fall Seasons

Temporal Allocation Issues (2)

- Facility vs. Process Differences
 - Each Unit At Plants Can Have Different Profile
- Area Sources Generally Use Default Profile
 - Ensure Appropriate Temporal Factors Used in Your Local Area
- Mobile Sources
 - Large Differences in Hour / Day / Week /Season Activity







Temporal Allocation Exercise (2)

■ From Seasonal Allocation Profiles

$$AF_{Win} = 0.075 + 0.075 + 0.075$$

 $AF_{Win} = 0.225$

Apply Winter Factor to Annual Emissions

 $E_{Win} = E_{Ann} * AF_{Win}$ $E_{Win} = 200 \text{ Tons VOC/yr} * 0.225$

 $E_{Win} = 45.0 \text{ Tons VOC}$

Temporal Allocation Exercise (3)

■ From Weekly Allocation Profiles

$$AF_{Sat} = (1/91) * (0.162/0.1429)$$

= 0.0125

Apply Saturday Factor to Season Emissions

 $E_{Sat} = E_{Win} * AF_{Sat}$

 $E_{Sat} = 45.0$ Tons VOC/Winter * 0.0125

 $E_{Sat} = 0.563$ Tons VOC/ Winter Saturday

Temporal Allocation Exercise (4)

■ From Hourly Allocation Profiles

$$AF_{9AM} = 0.071/1.00$$

= 0.071

Apply Hourly Factor to Daily Emissions

 $E_{9AM} = E_{Sat,Win} * AF_{9AM}$

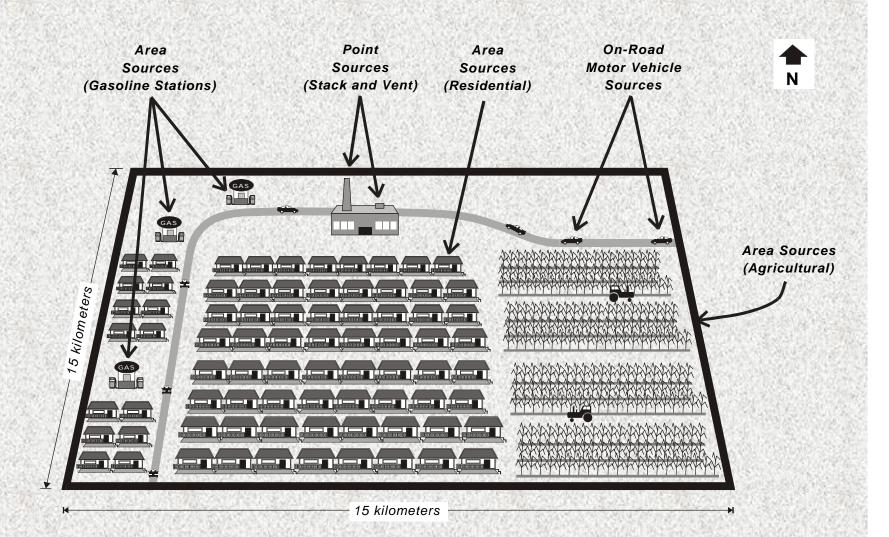
 $E_{9AM} = 0.563 \text{ Tons VOC} * 0.071$

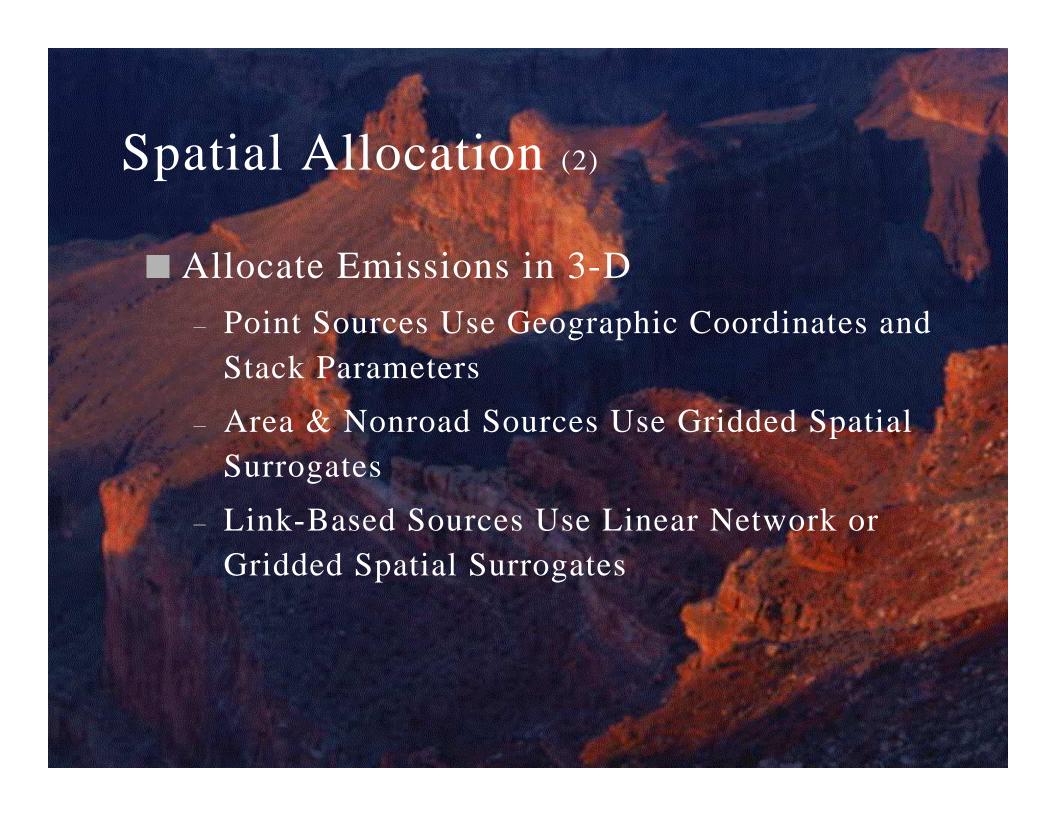
 $E_{9AM} = 0.040$ Tons VOC/ 9AM Winter Saturday

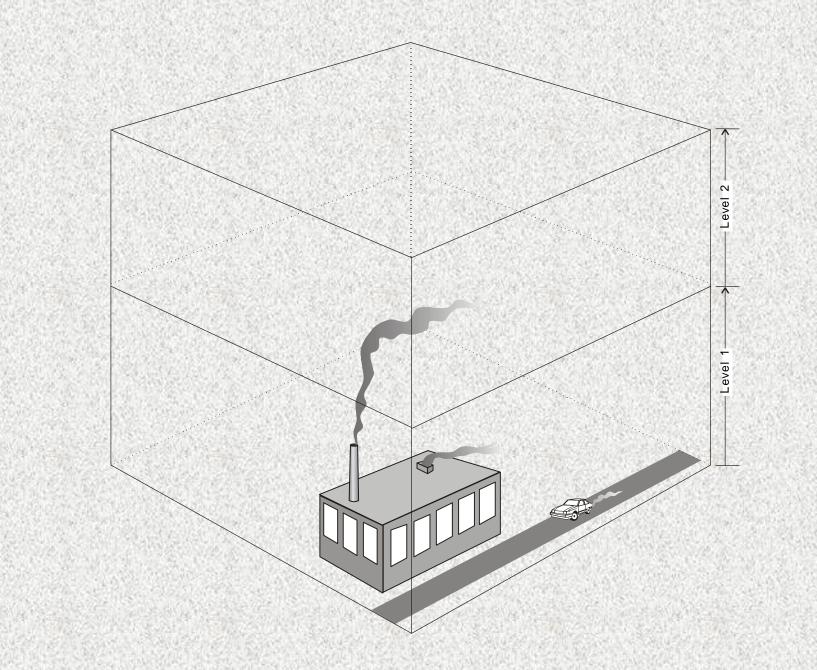


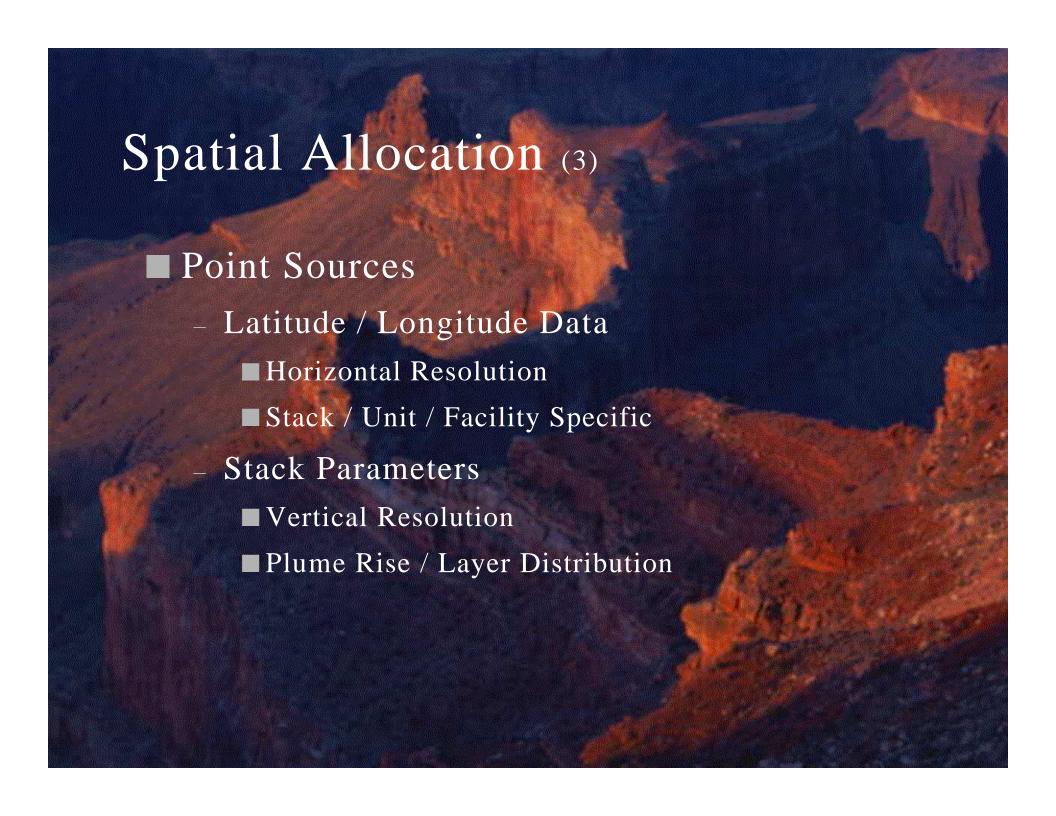
- Physical Location of Emission Sources
 - Emission Inventories Usually Provide Data At County or Census Tract Levels
 - Emission Models Use Allocation Ratios to
 Further Define Source Location
 - Modeling Objective Will Define Level
 - Local Scale Risk Exposure, Regional / National / International Transport Analyses

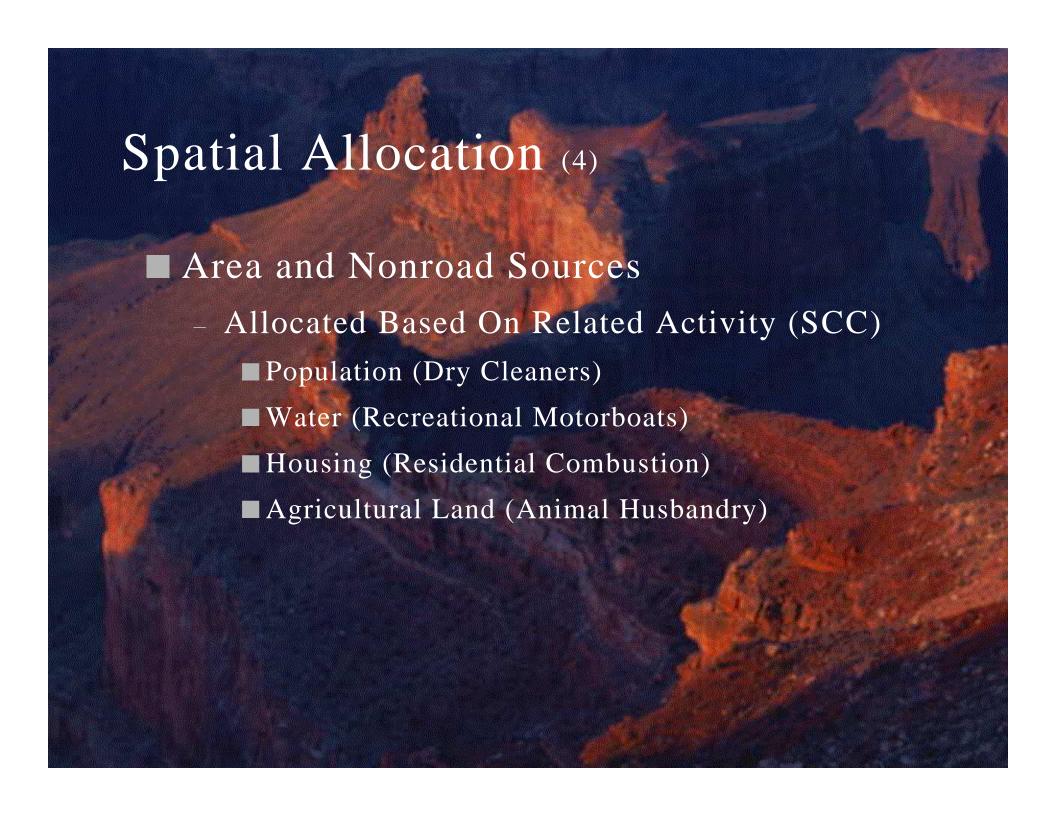
Example Modeling Domain

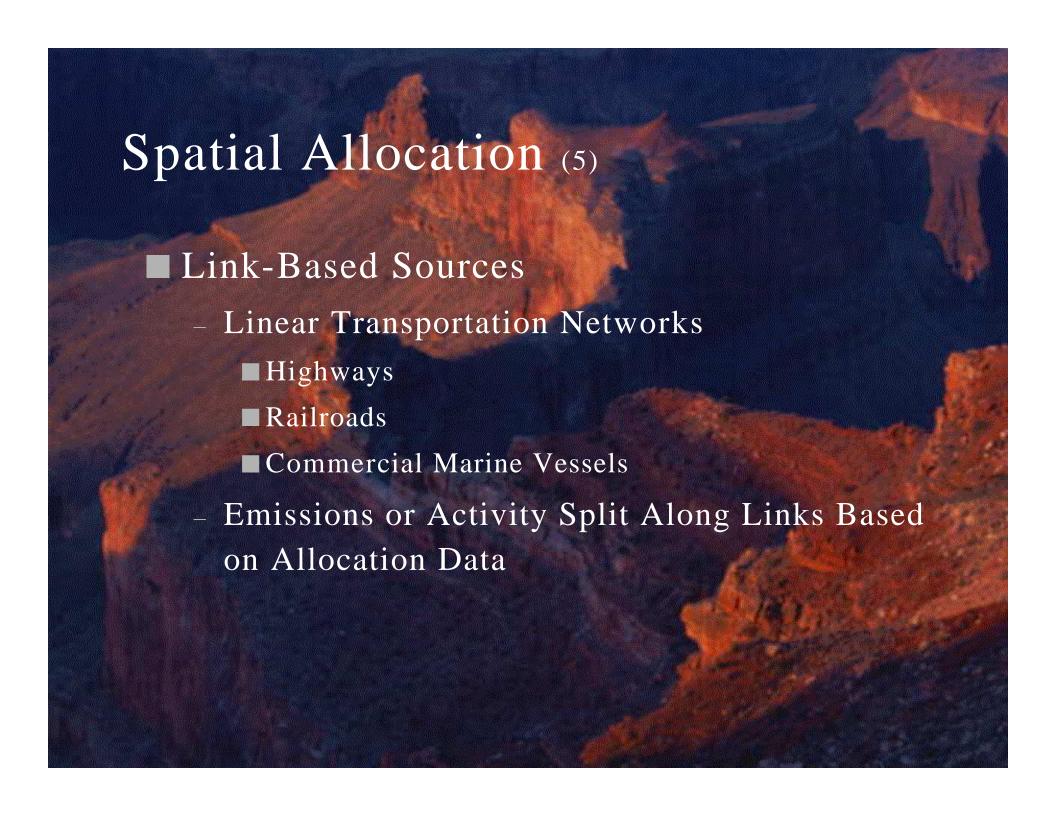


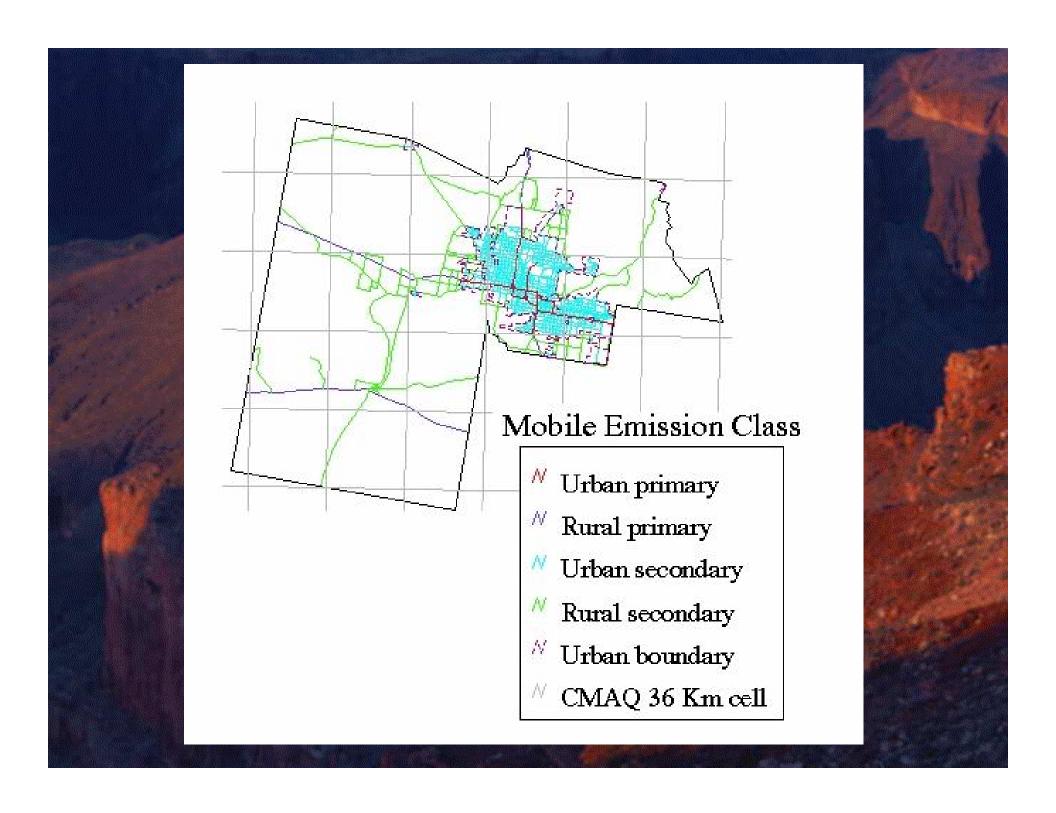










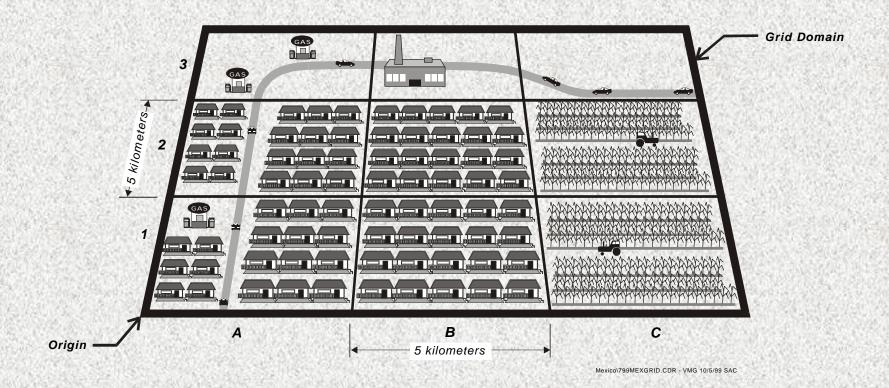


Spatial Allocation Ratios

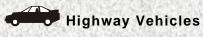
- Graphical Interface Systems (GIS) Used To
 Determine Gridding Ratio Information
 - Apply Surrogates To Site Emissions
 - Ratio of Grid Cell or Census Tract Contribution to Geographic Domain Emissions
 - Can Have Multiple Areas Within a Grid Cell
 - Usually Calculated Outside of Emissions Model

Example Gridded Domain





Example Spatial Ratios

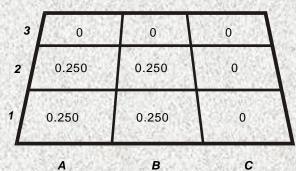


3	0.200	0.200	0.200	
2	0.200	0	0	
1	0.200	0	0	
	Δ	B	c	o e te

Gasoline Stations

3	0.667	0	0	
2	0	0	0	
1	0.333	0	0	
	Α	В	С	

Residential Consumer Solvent Use





Agricultural Pesticide Use

3	0	0	0
2	0	0	0.500
1	0	0	0.500

Spatial Allocation Example

■ Example:

 Calculate Annual VOC Emissions from Gasoline Stations in Grid Cell (A,1)

■ Steps:

- Estimate Grid Cell Allocation Factor from Gridding Profiles
- Apply Grid Cell Allocation Factor to Annual Emissions



■ Estimate Grid Cell Allocation Factor

 $AF_{Cell} = AC_{Cell} / AC_{Domain}$

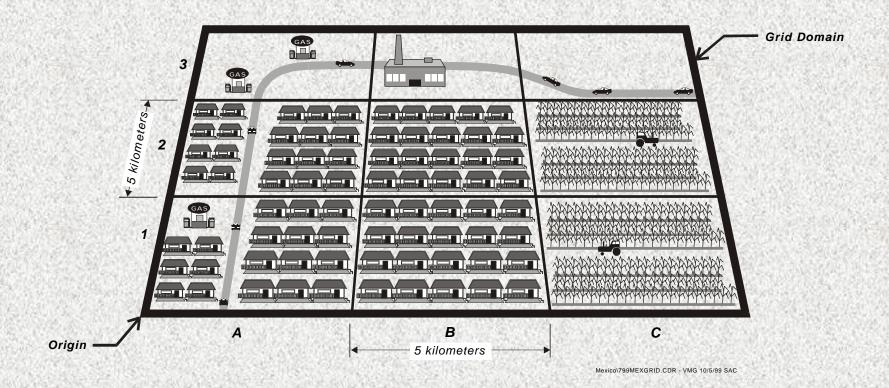
AF_{Cell} = Grid Cell Activity Factor

AC_{Cell} = Grid Cell Activity

AC_{Domain} = Domain Wide Activity

Example Gridded Domain





Spatial Allocation Example (3)

- From Gridded Domain Data
 - $-AF_{A,1} = 1$ Gas Station / 3 Gas Stations
 - $-AF_{A.1} = 0.333$
- Apply Gridding Factor to Annual Emissions

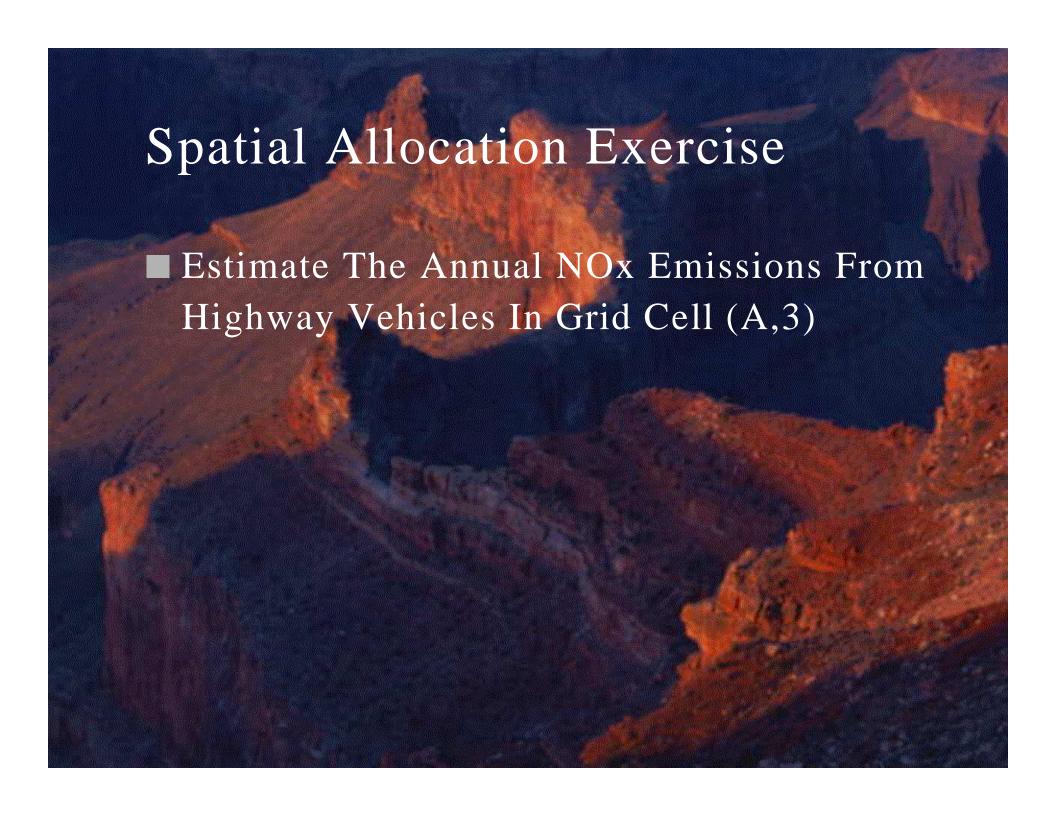
$$E_{A,1} = E_{Ann} * AF_{A,1}$$

 $E_{A,1} = 150 \text{ Tons VOC/year * } 0.333$

 $E_{A,1} = 50$ Tons VOC/year



- Ensure Lat/Lon Are In Proper County
 - No Sources In Lakes or Oceans
- Ensure Stacks Have Valid Data
 - No Supersonic Flow Rates
- Ensure Source and Roadway Types Are In Appropriate County
 - No Water, No Boats



Spatial Allocation Exercise (2)

■ From Example Spatial Ratios

$$-AF_{A,3} = 0.200$$

Apply Gridding Factor to Annual Emissions

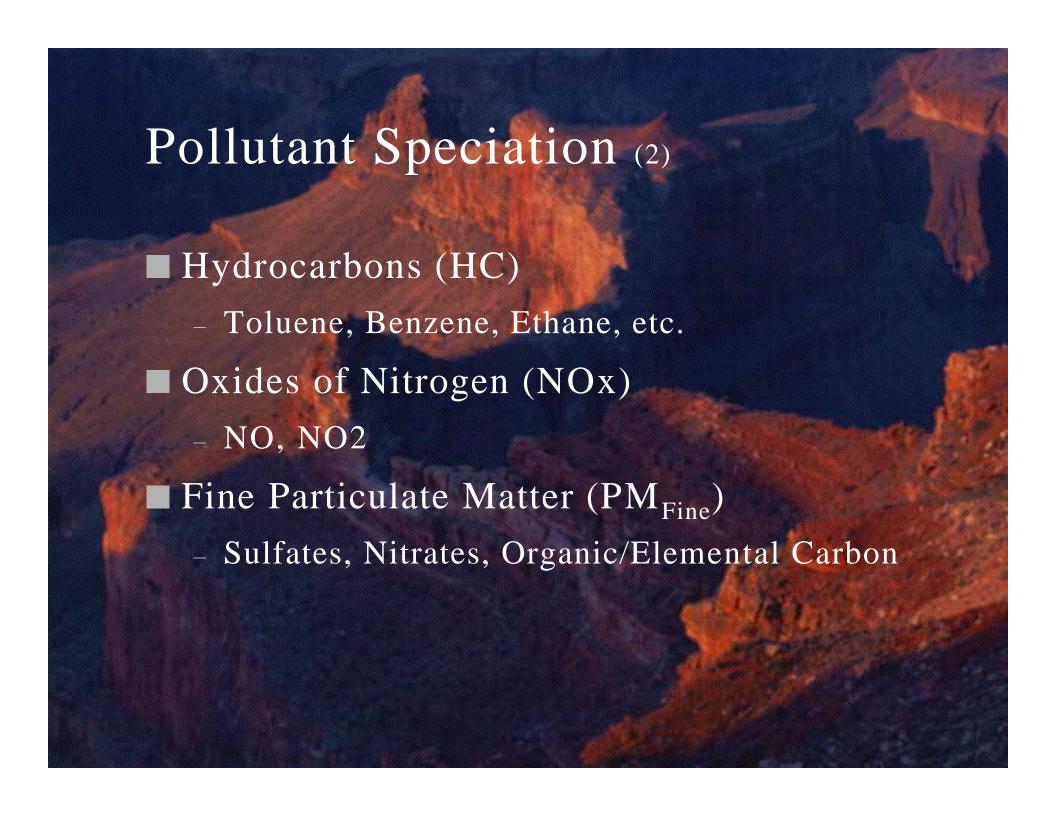
 $E_{A,3} = E_{Ann} * AF_{A,3}$

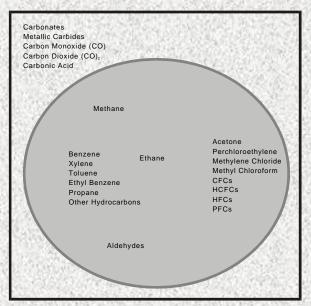
 $E_{A,3} = 800 \text{ Tons NOx/year} * 0.200$

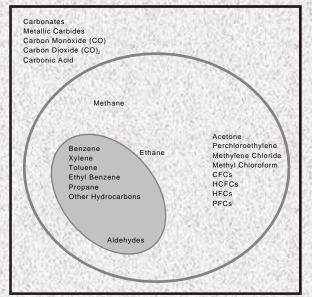
 $E_{A,3} = 160 \text{ Tons NOx/year}$

Pollutant Speciation

- Disaggregation of Pollutants Into Individual Chemical Species
 - Assign Speciation Profile to SCC
 - Determine Mass Fraction of Emitted Compounds
 - Determine Molecular Weight of Compound
- Used in Photochemical, Air Toxics, CMB, and Visibility Modeling

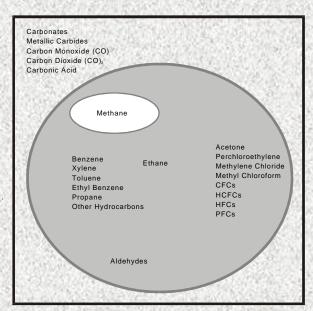


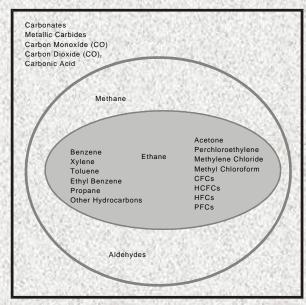


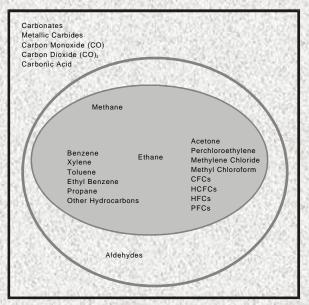


TOG/TOC

ROG/ROC/VOC

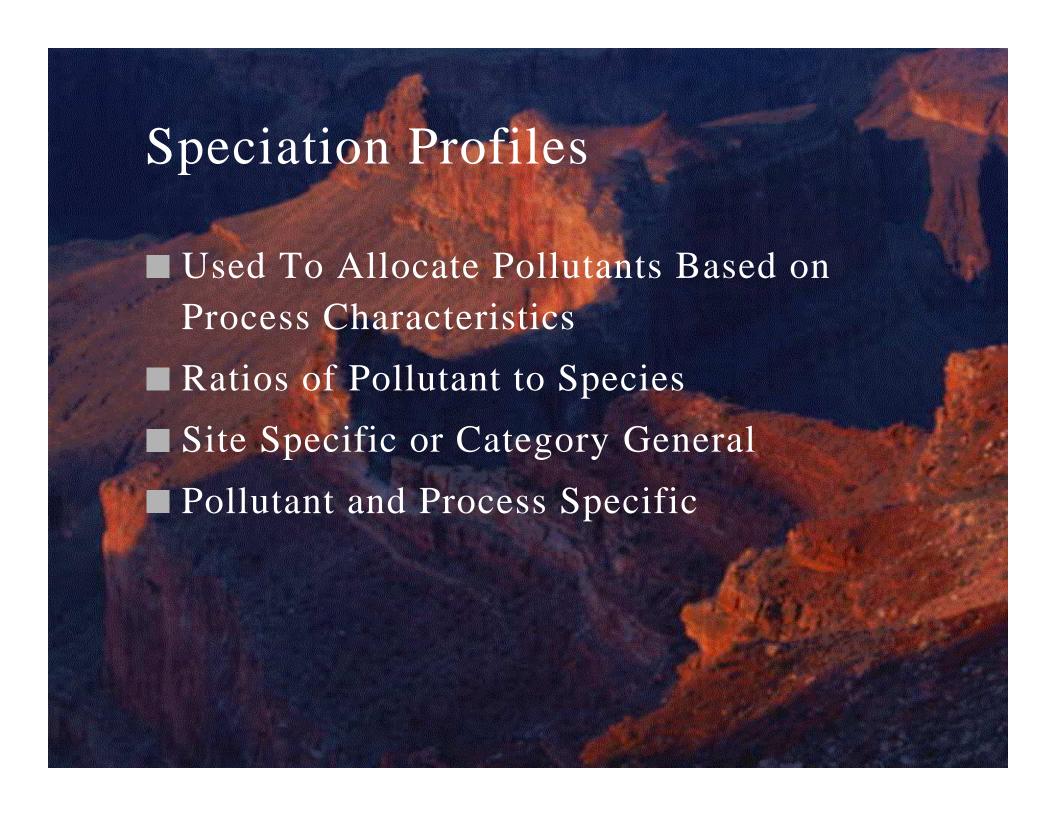






Photochemical Modeling

- Groups Species Into Chemical Mechanisms
- Defines Reactivity and Predictions of Pollutant Transformation
 - CB-IV
 - RADM
 - SAPRC99
- Occasionally Updated/Modified With Lab Study Data



VOC Speciation Profile Example

SCC Profile Assignment File

SCC	Profile
30101816	1004
30101817	1004
30101818	1004

Speciation Profile Example (2)

VOC Speciation Profile File

Profile	SAROAD	Mass Fraction
1003	98090	10.0015
1004	45203	0.1000
1004	45220	0.9000
1005	45220	1.0000

Speciation Profile Example (3)

Chemical Compound File

SAROAD	MW	Compund Name
	•••	
45202	92.14	Toluene
45203	106.17	Ethylbenzene
45204	106.17	O-Xylene
45218	134.22	M-Diethylbenzene
45220	104.15	Styrene
45221	118.18	Methylstyrene
The second secon		

Speciation Profile Example (4)

■ SCC 30101817: Emitting 20 Kg VOC / hour

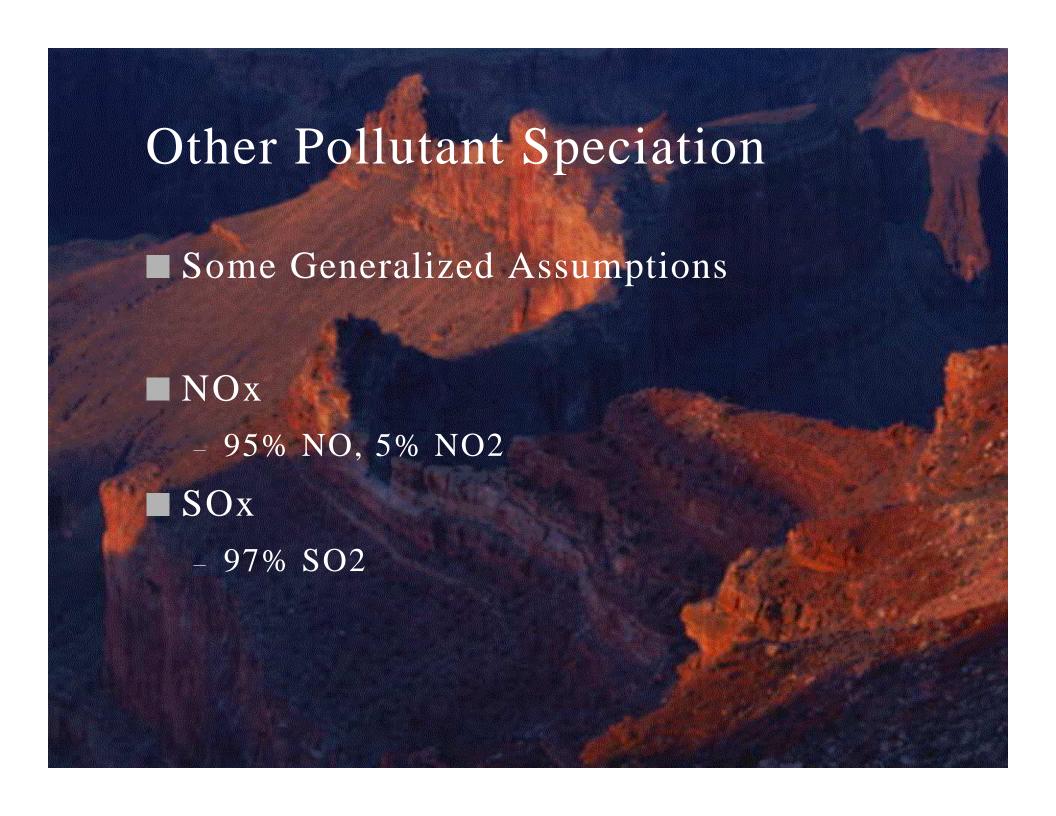
■ Mass Fraction

```
Q_{\text{ethylbenzene}} = 20 Kg/hr * 0.1000 = 2.0 Kg/hr

Q_{\text{styrene}} = 20 Kg/hr * 0.9000 = 18.0 Kg/hr
```

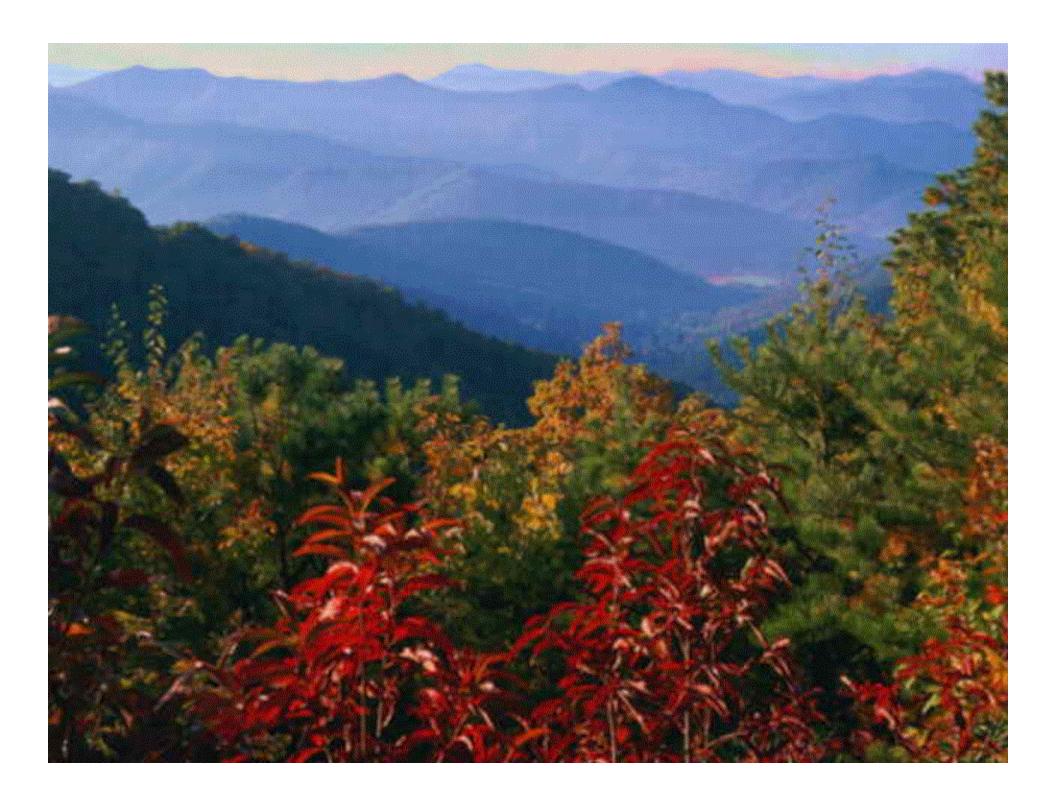
Molecular Weight

```
MW_{ethylbenzene} = 2.0 * 1000 g/Kg * (1g-mol/ 106.17 g) = 18.838 g-mol/hr
MW_{styrene} = 18.0 * 1000 g/Kg * (1g-mol/ 104.15 g) = 172.828 g-mol/hr
```



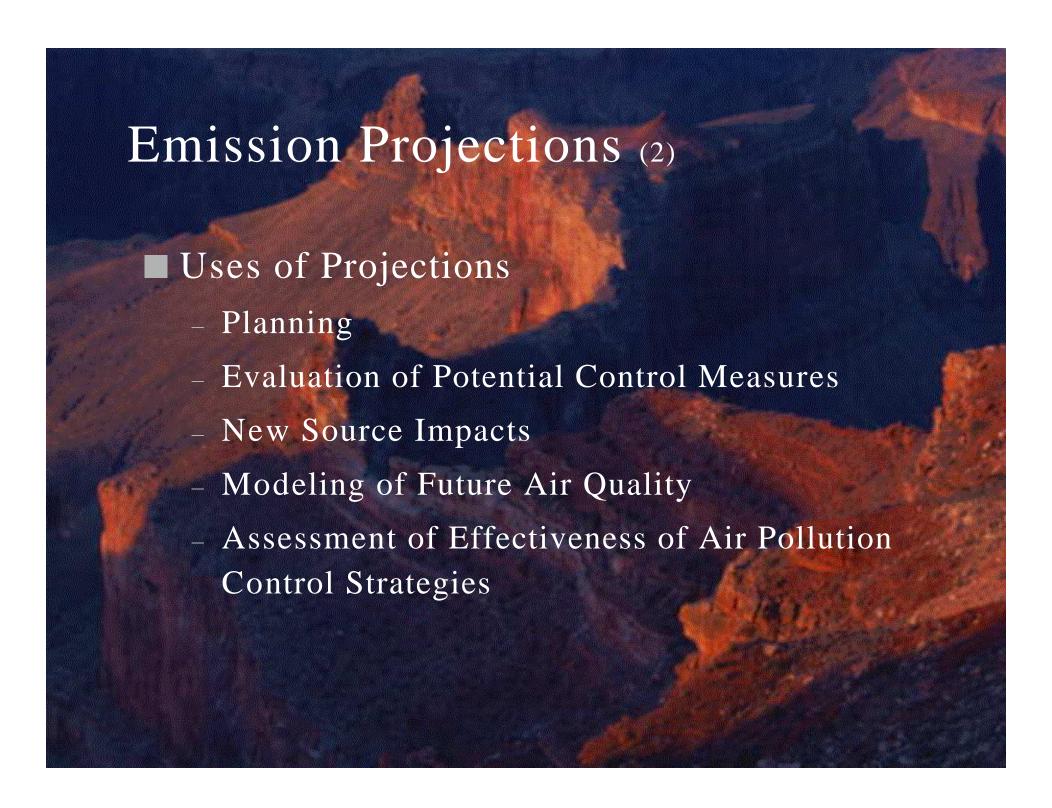
Chemical Speciation Issues

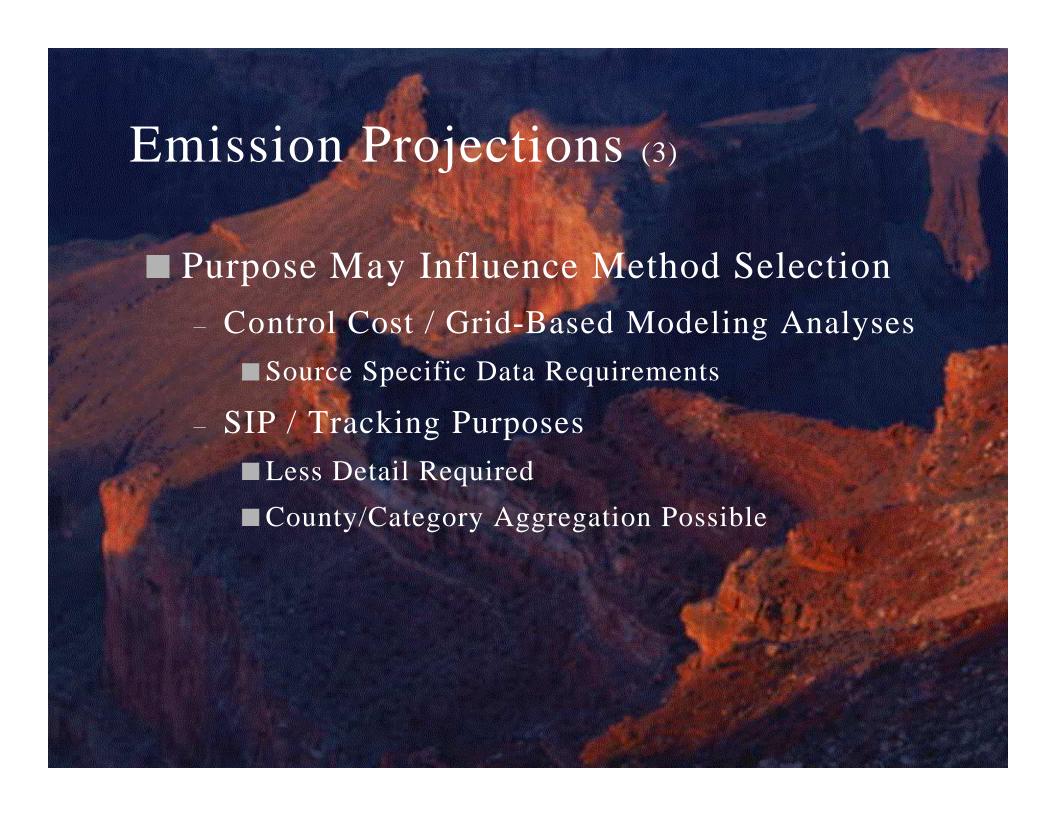
- VOC Speciated Emissions Are Not Comparable For Different Mechanisms
- Different Emission Processing Systems Are Likely To Use Different Profiles, Chemical Compound Data, and Mechanism Assignments
- Mechanism Speciation is Dependant on Chemical Compounds Identified in the VOC Speciation Profile
- Different Compound Names May Be Used by Various Mechanism Developers





- Extrapolation of Baseline Estimates
 - Future Activity Level Estimates
 - Future Expected Control
- Attempt to Predict and Quantify Unknown
 - Always Some Uncertainty in Projections
 - Goal Is To Minimize the Uncertainty





General Projection Equations

■ Emission Based

$$E_{fy} = E_{by} * GF * CF$$

 E_{fv} = Projection Year Emissions

 E_{bv} = Base Year Emissions

GF = Growth Factor

CF = Control Factor

General Projection Equations (2)

Activity Based

$$E_{fy} = A_{by} * GF * EMF_{fy}$$

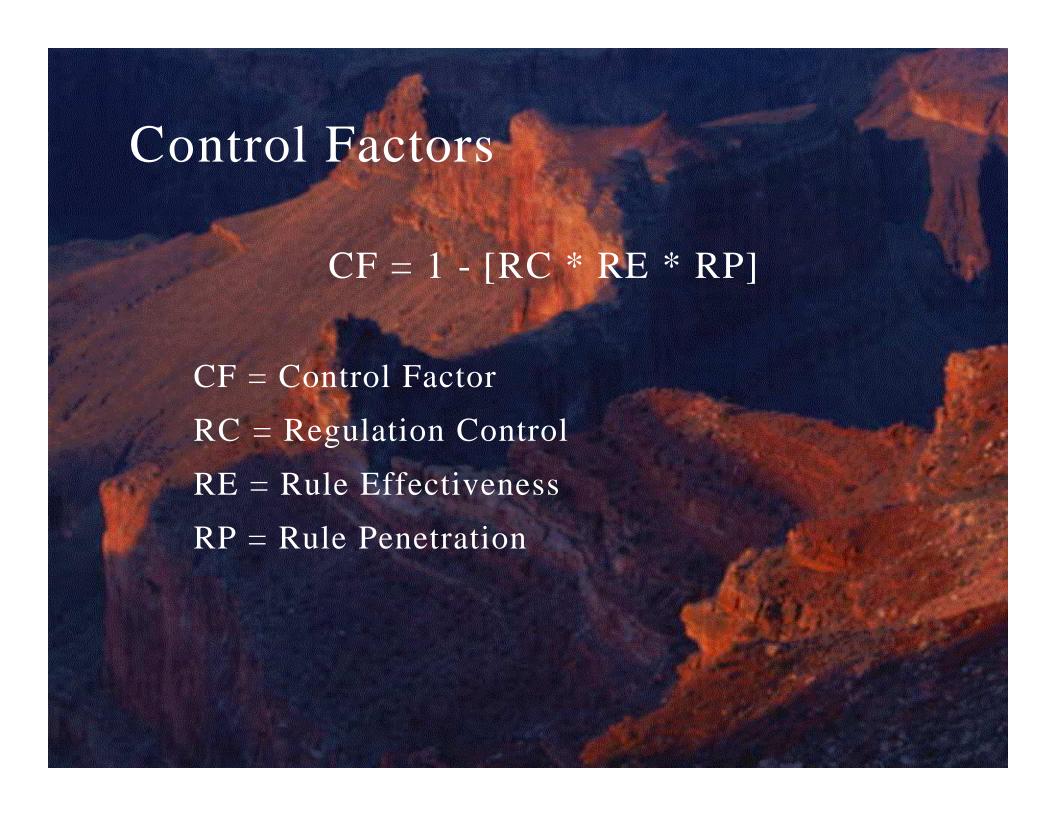
E_{fy} = Projection Year Emissions

 A_{bv} = Base Year Activity

GF = Growth Factor

EMF_{fy} = Projection Year Emission Factor







- Regulation Control
 - Expected Reduction For Control Measure
- Rule Effectiveness
 - Regulatory Program Effectiveness
 - Regulation, Compliance, Performance of Regulation
- Rule Penetration
 - Quantifies Regulation's Coverage of Category



- Estimates of Future Year Emissions that Include Expected Impact of Modified or Additional Control Regulations
 - Fuel Switching, Fuel Efficiency Improvements
 - Pollution Prevention Programs
 - Greenhouse Gas or Global Warming Initiatives



- Model Develops Projections
 - Base Year Inventory
 - Growth Factors
 - Control Factors
- Develop Projections Outside Model
 - Input Projected Inventory in Same Format as Base Year Inventory

Emission Projection Example

■ Example:

Calculate Annual CO Emissions from Factory
 Boiler Assuming 25 % Growth, No Existing
 Control, 40 % Regulation Control, 100 % Rule
 Effectiveness, and 100 % Rule Penetration

■ Steps:

- Estimate Control Factor for Process
- Apply Growth and Control To Base Emissions

Emission Projection Example (2)

■ Estimate Control Factor for Process

CF = 1 - [RC * RE * RP]

CF = 1 - [(40/100) * (100/100) * (100/100)]

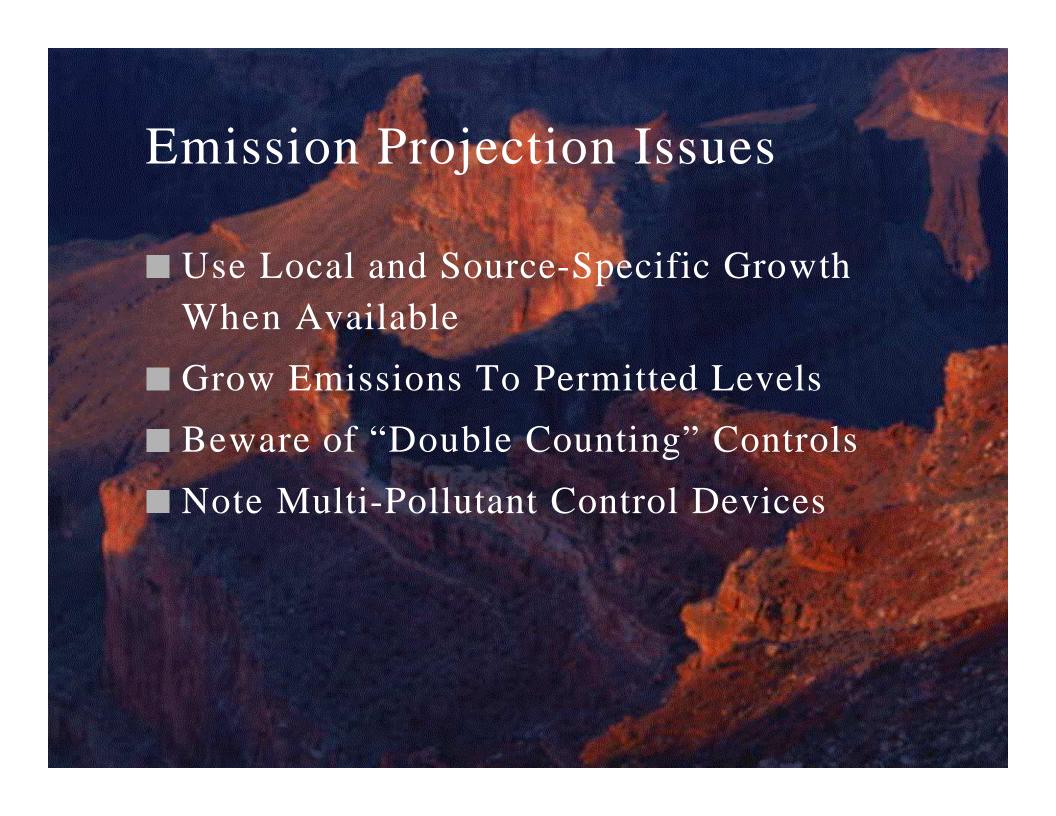
CF = 1 - 0.40

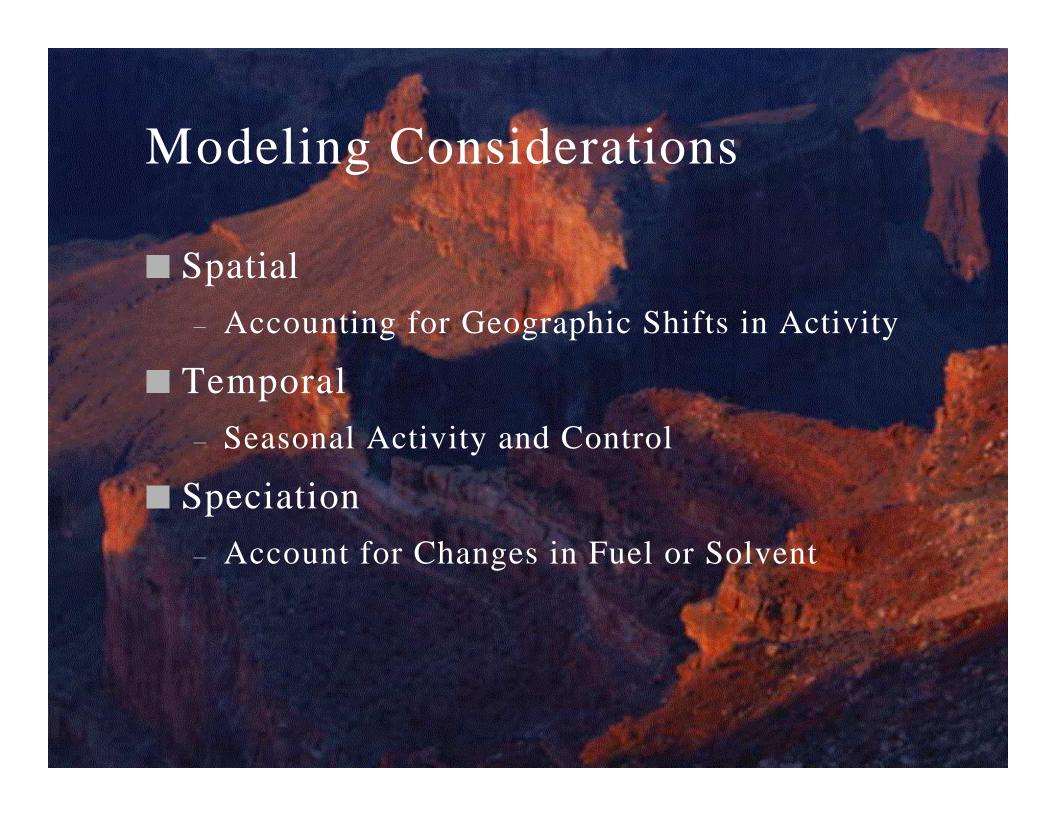
CF = 0.60 or 60%



Apply Growth and Control To Base Emissions

 $E_{fy} = E_{by} * GF * CF$ $E_{fy} = 600 \text{ tpy CO} * 1.25 * 0.60$ $E_{fy} = 450 \text{ tpy CO}$







- Estimate The Annual VOC Emissions From Agricultural Pesticide Application Assuming The Following:
 - Growth Rate = 50 %
 - Regulation Control = 25 %
 - Rule Effectiveness = 100 %
 - Rule Penetration = 50 %

Emission Projection Exercise (2)

■ Estimate Control Factor for Process

CF = 1 - [RC * RE * RP]

CF = 1 - [(25/100) * (100/100) * (50/100)]

CF = 1 - 0.125

CF = 0.875 or 87.5%

Emission Projection Exercise (3)

Apply Growth and Control To Base Emissions

 $E_{fy} = E_{by} * GF * CF$

 $E_{fv} = 100 \text{ tpy VOC} * 1.50 * 0.875$

 $E_{fy} = 131.25 \text{ tpy VOC}$



- Some Models Used To Estimate Emissions
 - Nonroad Sources
 - Highway Vehicles
 - Biogenic Emissions
- Account For Episode Specific Data
 - Temperatures, Precipitation, Cloud Cover, etc.

Nonroad Emissions Modeling

- EPA's NONROAD Model for Most Nonroad Sources
 - Exception Airport, Commercial Marine, Railroad
- Use Local Data Where Available
- Make Sure New Nonroad SCCs are Incorporated into Emission Model
 - Spatial Surrogates
 - Temporal and Speciation Profiles

Highway Emissions Modeling

- Ozone Modeling
 - Episode Specific Hourly Emissions
 - Needed Inputs
 - Vehicle Miles Traveled
 - MOBILE Model Input Shells
 - Vehicle Speeds
- PM or Air Toxics Modeling
 - Precaclulated and Treated as Area Sources

